

Ethyl 4-ethoxybutyrate

26448-91-9 | DTXSID10403149

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 9.40e-01

Global applicability domain: Inside

Local applicability domain index: 5.58e-01

Confidence level: 7.21e-01

Nearest Neighbors from the Training Set

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Paraldehyde

Measured: 0.67

Predicted: 8.50e-01

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Ethyl orthoformate

Measured: 1.20

Predicted: 1.05

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1-Methoxy-2-propyl acetate

Measured: 0.56

Predicted: 4.87e-01

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Methyl pivalate

Measured: 1.83

Predicted: 1.76

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2,2-Dimethyl-1,3-dioxolane

Measured: 0.46

Predicted: 5.11e-01